BIOGRAPHICAL SKETCH

NAME	POSITION TITLE
Michael-Rock Goldsmith, Ph.D.	**Chemist**
eRA COMMONS USER NAME	

EDUCATION/TRAINING

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)	FIELD OF STUDY
Marianopolis College, Montreal QC Canada	D.E.C.	1993-1995	Health Sciences
Concordia University, Montreal QC Canada	B.Sc.	1995-1998	Chemistry
Duke University, Durham NC	Certificate	2003-2005	Structural Biology & Biophysics
Duke University, Durham NC	Ph.D.	2000-2005	Theoretical Chemistry
UNC-Chapel Hill, School of Public Health	Postdoctoral trainee	2006-2007	Computational Toxicology in DESE

A. POSITIONS and HONORS

Research and Professional Experience:

2007-Present *Postdoctoral trainee*, R-Authority / Cross-ORD Postdoctoral Fellow working at the National Center for Computational Toxicology, Office of Research and Development, **U.S. EPA**
2006-2007 *Postdoctoral trainee*, **UNC-CH (SPH/DESE)** working at the National Center for Computational Toxicology, Office of Research and Development, **U.S. EPA**
2006 Physiologically-Based Pharmacokinetic Modeling *Trainee*, CIIT, NC
2001-2005 *Research Assistant*, Chemistry Department, **Duke University**
2000-2001 *Research Assistant*, Chemistry Department, **University of Pittsburgh**
1999-2000 *Analyst*, PR&D/QA, **Ethypharm DDS Inc.**
1999 *QA Analyst*, PR&D, **Pharmascience**
1999 *Analyst*, Quality Assurance, **Novartis Pharma Canada**
1998* *Jr. Formulation Scientist*, **Emulsion Explosives Group, ICI/Orica Canada**
1997* *Scientist*, Product Engineering, **Imperial Tobacco Inc.**
1997* *Jr. Analytical Chemist, Pharmaceutical R&D*, **Merck-Frosst Canada**
1996* *Analyst*, Quality Assurance, **Ciba-Geigy Canada**
*= CO-OP work-terms

Professional Societies and Affiliations:

American Chemical Society – Full Member	2000-Present
Society of Toxicology – Full Member	2006-Present
Triangle Reproductive Biology Consortium	2006-Present
US-EPA Networking & Leadership Trainee Organization – RTP	2006-Present

Honors and Awards:

Recipient of a US-EPA – HEASD ***"on the spot" award*** for work on modeling stereoselectivity of chiral pyrethroids performed in conjunction with D. Chang and C. Dary (US-EPA LV)
Graduate Student Travel Grant (2004- APS, Montreal / 2003- SETCA, Clemson).
Aristech Fellowship - University of Pittsburgh (2000) & Chair's Scholar Grant (2000).
Two-time recipient of Canadian NSERC Industrial Undergraduate Student Research Awards (USRA) (1998 ICI-Explosives, 1997 Merck-Frosst).
Graduated with Distinction from Concordia University's Chemistry Co-operative Education Program and member of Honours Program (1995-1998).

Selected Invitations at National & International Symposia:

A Virtual High-Throughput Screening and Docking Workshop – National Institute of Statistical Science, 11/28/2007, organized by SimBioSys http://www.simbiosys.ca/science/presentations/2007-11-RTP/RTP_Seminar_Nov28_NISS_agenda.html

Bio-Tools Vibrational Circular Dichroism Get-Together – November 2007, Somerset NJ

PFAA Reunion — August 2007, RTF/ US-EPA, RTP NC

Goldsmith, M-.R.; Chang, D.; Tornero-Velez, R.; Little, S. B.; Rabinowitz, J., Curtis, D.; *An in silico consensus docking approach towards elucidating the stereoselectivity of pyrethroid-like compounds in carboxylesterase*. 2007, ICT-IuTox Montreal.

Goldsmith, M-.R.; Little, S. B.; Reif, D.; Rabinowitz, J.R..; Digging Deeper into Deep Data: Molecular Docking as a Hypothesis-driven Biophysical Interrogation System in Computational Toxicology. 2007, International Science Forum.

Goldsmith, M-.R.; Little, S. B.; Reif, D.; Goetz, A. K.; Rabinowitz, J.R..; *Biophysical Models in Modern Risk Assessment: Conazoles in the Human Context.* 2007, Society of Biomolecular Screening, Montreal..

Goldsmith, M-.R.; Little, S. B.; Reif, D.; Rabinowitz, J.R..; *Structure-Guided Virtual High-Throughput Screening Prioritization Models: Nuclear Receptors and Environmental Chemicals*. 2007, SOT Charlotte, NC.

Goldsmith, M-R. *Twisted Tail of a Narcissistic Molecule: Biophysical Modeling and Meta-Analysis of Fluorous Chemicals in the Biological Milieu.* RTD seminar series, Reprotductive Toxciology Facility US-EPA NC.

Goldsmith, M-.R.; Little, S. B.; Rabinowitz, J.R.; *Molecular Models of Environmentally Persistent Perfluorinated Chemicals in the Biological Milieu*. 2007, CCT SOT, Arlington VA.

Goldsmith MR, Little S, Rabinowitz J. *Macromolecular Target for Chemical Toxicity: Models of the Interactions of Peroxisome Proliferator Activated Receptors with Perfluorinated Organic Compounds.* National Center for Computational Toxicology /US-EPA BOSC June 2006 & at the US-EPA Endocrine Disrupting Workshop July 2006 both in RTP, NC.

Pasquinelli MA, Little S, Goldsmith MR, Rabinowitz J. *Molecular Modeling as a Tool for Understanding human health Risks.* US-EPA Science Forum 2006 (Washington, DC)

Goldsmith MR. *Probing the structure of dynamic biologically relevant molecules through theory: QM and classical approaches*. National Center for Computational Toxicology, US-EPA (RTP, NC) October 2005

Goldsmith MR, Prytkova T, Beratan DN, McGowan L. *Modeling the Temperature-Dependent Aptamer-Peptide Specificity*. Triangle Biophysics Symposium, NC, November 2004.

Goldsmith MR, George CB, Zuber G. Naaman R, Waldeck. DH, Wipf P, Beratan DN *Chiroptic Signatures of Thiol-Passivated Nanoclusters: A Theoretical Approach.* SERMACS, November 2004 (RTP, NC)

Zuber G, Goldsmith MR, Beratan DN, Wipf P. *Assignment of Absolute Configuration of the Natural Product Bistramide A using TDDFT Optical Rotation*. SERMACS, November 2004 (RTP, NC)

Goldsmith MR, George CB, Zuber G. Naaman R, Waldeck. DH, Wipf P, Beratan DN *Chiral Image-Charges in Nanoclusters.* APS conference – Montreal,March 2004 *Awarded Duke Graduate Travel Grant

Goldsmith MR, Beratan DN, Wipf P. *Chiroptics of Assemblies*. SETCA 2003 March 2003* (Clemson, SC) *Awarded Duke Graduate Travel Grant

Goldsmith MR, Beratan DN, Wipf P. *Optical Activity in Dimers and Aggregates*. Duke Biochemistry Retreat - Boone, NC.

Goldsmith MR. *Exploiting Bananas for Novel Materials and Electro-Optical Devices*. Duke University Seminar Series 2002.

Goldsmith MR, Beratan DN, Wipf P. *Optical Activity in Dimers and Aggregates*. Gordon Research Conference – Stereochemistry, Newport, RI 2002.

Selected Expert Committees/Advisory Panels/Organizing Committees:

Contributing research to Pyrethroid safety assessment for predictive metabolism

Organized a two-day training event for NCCT for practical use of Chemical Computing Group's Molecular Operating Environment (MOE) at the National Computing Center.

Member of the US-EPA Networking and Leadership Trainee Organization (2006-2007) – organized Science Forum 2007 post-doc social

Multiple NCCT, US-EPA post-doc, and Science-Forum 2007 web-site and graphics contributions.

Selected Assistance/Advisory Support to the Agency:

Design and Implementation of a multi-target virtual screening infrastructure in collaboration with Lockheed-Martin Contractors and assistance in establishing collaboration with SimBioSys on Large-Scale Virtual Screening Project - http://www.simbiosys.ca/whatsnew/news/index.html#20071105

Benchmarked external distributed computing infrastructure for production mode docking on the SunGrid (Sun Microsystems) with Simbiosys eHiTS software. http://www.simbiosys.ca/whatsnew/newsletter/2007-03.html#eHiTS_available_in_the_Application

Organized a two-day training event for NCCT for practical use of Chemical Computing Group's Molecular Operating Environment (MOE).

Requested by other Laboratories to assist in NCCU virtual screening demo for CompTox tour.

B. SELECTED PUBLICATIONS

Goldsmith, M-.R.; Chang, D.; Tornero-Velez, R.; Little, S. B.; Rabinowitz, J., Curtis, D.; Structure-Based Models for Estimating Kinetic Parameters of Stereoselective Enzymatic Hydrolysis of Chiral pyrethroids by Human Carboxylesterase. **2007**, *submitted 2007*.

Rabinowitz, J. R.; Goldsmith, M.-R.; Little, S. B.; Pasquinelli, M. A.; Prioritizing Bioassay Requirements for Environmental Chemicals; Applications of Computational Molecular Models for Macromolecular Targets of Chemical Toxicity. **2007**, *submitted to EHP 11/2007*

Mukhopadhyay, P.; Zuber, G.; Goldsmith, M-.R.; Wipf, P.; Beratan, D. N.; Solvent Effect on Optical Rotation: a Case Study of Methyloxirane in Water. *ChemPhysChem*, **2006**, 7, 2483-2486.

Perry, J. L.; Goldsmith, M. R.; Williams, T. R.; Radick, K.; Christenson, T.; Gorham, J.; Pasquinelli, M. A.; Toone, E. J.; Beratan, D. N.; Simon, J. D.; Binding of Warfarin Influences the Acid-Base Equilibrium of H242 in Sudlow Site I of Human Serum Albumin.; *Photochem Photobiol*. **2006**, 82, 1365-1369.

Goldsmith, M.-R., George C. B., Zuber, G.; Naaman, R.; Waldeck. D. H., Wipf, P.; Beratan D. N. The chiroptical Signature of Achiral Metal Clusters induced by Dissymetric Adsorbates. *Phys. Chem. Chem. Phys.* **2006**, 8, 63-67.

Simon J. D.; Goldsmith, M.-R.; Hong, L.; Kempf, V.L.; McGuckin, L. E.L.; Ye,T.; Zuber, G. Spectroscopy and Photoreactivity of Trichochromes: Molecular Components of Pheomelanins Photochem Photobiol. **2006**, 82(1), 318-323.

Zuber, G.; Goldsmith, M.-R.; Hopkins, T. D.; Beratan, D. N.; Wipf, P. Systematic Assignment of the Configuration of Flexible Natural Products by Spectroscopic and Computational Methods: The Bistramide C Analysis. *Org. Lett*. **2005**, 7(23), 5269-5272.

Zuber, G.; Goldsmith, M.-R.; Beratan, D. N.; Wipf, P. Assignment of the absolute configuration of [n]-ladderanes by TD-DFT optical rotation calculations. *Chirality* **2005**, 17(8), 507-510.

Zuber, G.; Goldsmith, M.-R.; Beratan, D. N.; Wipf, P. Towards Raman optical activity calculations of large molecules. *ChemPhysChem* **2005**, 6(4), 595-597.

Goldsmith, M. R; Perry, J. L.; Peterson, M. A.; Beratan, D. N.; Wozniak, G.; Rueker, F.; Simon, J. D. Structure of the Ochratoxin A Binding Site within Human Serum Albumin. *J. Phys. Chem. B* **2004**, 108(43), 16960-16964.

Goldsmith, M.-R.; Jayasuriya, N.; Beratan, D. N.; Wipf, P. Optical Rotation of Noncovalent Aggregates. *J. Am. Chem. Soc.* **2003**, 125(51), 15696-15697.

Perry, J. L.; Christensen, T.; Goldsmith, M.-R..; Toone, E. J.; Beratan, D. N.; Simon, J. D. Binding of Ochratoxin A to Human Serum Albumin Stabilized by a Protein-Ligand Ion Pair. *J. Phys. Chem. B* **2003**, 107(31), 7884-7888.